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The flux synthesis of single crystals of the isostructural compounds tristrontium zinc platinum hexaoxide, Sr_3ZnPtO_6, and tristrontium cadmium platinum hexaoxide, Sr_3CdPtO_6, is reported. The compounds adopt the pseudo-one-dimensional rhombohedral K_4CdCl_6 structure type, and feature chains of face-shared distorted ZnO_6 or CdO_6 trigonal prisms and PtO_6 octahedra, surrounded by columns of Sr^{2+} ions. All transition metals are located on the threefold axis of symmetry, while the Sr^{2+} cations lie on twofold axes.

Comment

Interest in detailed structural and magnetic measurements on oxides adopting the K_4CdCl_6 structure type (Bergerhoff & Schmitz-Dumont, 1956) has been great during recent years, mostly due to the low-dimensional nature and compositional flexibility of this large class of oxides. Though the work to date has involved predominantly powder studies, a few single-crystal studies of platinates of this type have been reported, beginning with Sr_4PtO_6 in 1959 (Randall & Katz, 1959) and

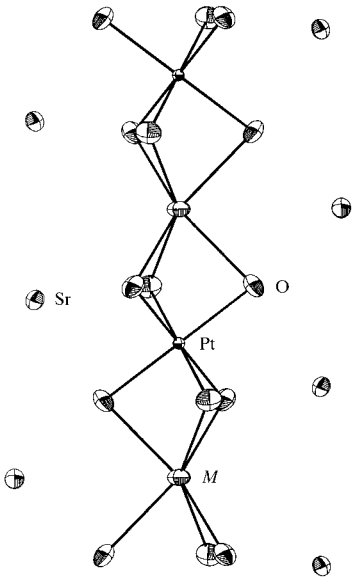

Figure 1
A section of the face-shared $MPtO_6$ (M is Zn or Cd) chains in the title compounds. Displacement ellipsoids are drawn (M = Cd) at the 80% probability level.

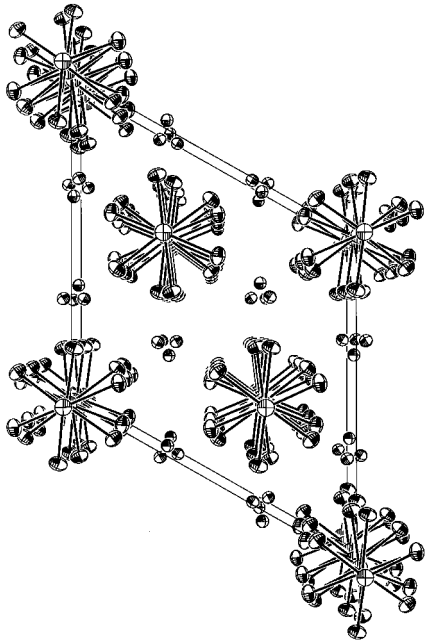

Figure 2
A view of Sr_3MPtO_6 (M is Zn or Cd) along [001].

including Sr_3CuPtO_6 (Wilkinson *et al.*, 1991), Sr_3NiPtO_6 (Nguyen *et al.*, 1997) and Ca_4PtO_6 (Claridge *et al.*, 1997). During the course of investigations into preparing single crystals of compositions related to Sr_3MPtO_6, we have grown single crystals of Sr_3ZnPtO_6, (I), and Sr_3CdPtO_6, (II), from potassium hydroxide fluxes at high temperatures, employing the Pt^{4+}-containing precursor $(NH_4)_2PtCl_6$. While (I) has been determined previously by X-ray powder diffraction (Lampe-Önnerud & zur Loye, 1996), (II) has not been reported.

The structures of the title compounds consist of chains of slightly distorted face-shared ZnO_6 [in (I)] or CdO_6 [in (II)] trigonal prisms which alternate with rhombohedrally elongated PtO_6 octahedra along [001] (Fig. 1). The distortion of the trigonal prisms consists of a rotation of the opposite triangular faces away from ideal eclipsed geometry [12.3° for (I) and 13.6° for (II)]. The chains are surrounded by six spiral columns of Sr^{2+} ions, and the Sr^{2+} columns are in turn surrounded by three polyhedral chains (Fig. 2). The Sr^{2+} ions occupy an irregular eight-coordinate position, just off the threefold axis on a position of site symmetry 2.

The Zn—O bond distance in (I) is essentially identical to the value determined previously from powder data [2.199 (4) Å; Lampe-Önnerud & zur Loye, 1996]. The Cd—O distance in (II) also agrees with the few known bond lengths for Cd in a trigonal prismatic coordination, *i.e.* 2.302 (6) Å in Sr_3CdIrO_6 (Segal *et al.*, 1996) and 2.338 (4) Å in Sr_3CdRhO_6 (Smith & zur Loye, 2000). The Pt—O distances (Tables 1 and 2) in both compounds are typical of octahedral Pt^{4+} in platinates.

Experimental

$(NH_4)_2PtCl_6$ was prepared according to Kaufman (1967). Subsequently, $SrCO_3$ (Alfa, 99.95%), ZnO (Alfa, 99.99%) or CdO (Alfa, 99.99%), and $(NH_4)_2PtCl_6$ (stoichiometric amounts, *ca* 1 g total reagent mass) and KOH (Fisher, reagent grade; ~10 times by mass the total reagent amount) were loaded into a covered alumina

Table 1
Selected geometric parameters (Å) for (I).

Sr—O^{i}	2.476 (4) × 2	Zn—O	2.200 (4) × 6
Sr—O^{ii}	2.645 (4) × 2	Zn—Pt	2.8073 (3) × 2
Sr—O^{iii}	2.668 (4) × 2	Pt—O	2.029 (4) × 6
Sr—O^{iv}	2.718 (4) × 2		

Symmetry codes: (i) $-x+y, -x, z$; (ii) $\frac{2}{3}+x-y, \frac{1}{3}+x, \frac{1}{3}-z$; (iii) $\frac{2}{3}-y, \frac{1}{3}+x-y, \frac{1}{3}+z$; (iv) $\frac{2}{3}-x, \frac{1}{3}-y, \frac{1}{3}-z$.

crucible. The mixture was heated at 1273 K for 2 h and cooled to 1023 K at a rate of 1 K h^{-1}, at which point the furnace was shut off and allowed to cool radiatively to room temperature. The KOH matrix was dissolved with distilled water, leaving numerous blue–green hexagonal prisms and less abundant brown crystals with a rhombohedral habit. Both morphologies were determined to be rhombohedral Sr_3MPtO_6 by powder X-ray diffraction. However, all of the blue–green hexagonal rods displayed obverse–reverse rhombohedral twinning, and therefore the brown crystals were selected for analysis.

Compound (I)

Crystal data

Sr_3ZnPtO_6
M_r = 619.32
Trigonal, $R\bar{3}c$
a = 9.6267 (7) Å
c = 11.2292 (11) Å
V = 901.23 (13) Å^3
Z = 6
D_x = 6.847 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 823 reflections
θ = 4.23–36.20°
μ = 53.564 mm^{-1}
T = 293 (2) K
Fragment, brown
0.11 × 0.05 × 0.03 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.054, T_{max} = 0.211
2881 measured reflections
493 independent reflections
R_{int} = 0.045
θ_{max} = 36.32°
$h = -13 \rightarrow 15$
$k = -13 \rightarrow 15$
$l = -18 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.059
S = 0.981
493 reflections
20 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0272P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 6.49 e Å^{-3}
$\Delta\rho_{min}$ = −4.57 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.00027 (5)

Compound (II)

Crystal data

Sr_3CdPtO_6
M_r = 666.35
Trigonal, $R\bar{3}c$
a = 9.6413 (4) Å
c = 11.5935 (7) Å
V = 933.29 (8) Å^3
Z = 6
D_x = 7.114 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1517 reflections
θ = 4.23–36.22°
μ = 51.286 mm^{-1}
T = 293 (2) K
Chunk, brown
0.09 × 0.04 × 0.03 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.091, T_{max} = 0.360
2632 measured reflections
505 independent reflections
R_{int} = 0.036
θ_{max} = 36.35°
$h = -15 \rightarrow 8$
$k = -16 \rightarrow 15$
$l = -19 \rightarrow 9$

Table 2
Selected geometric parameters (Å) for (II).

Sr—O^{i}	2.529 (4) × 2	Cd—O	2.328 (4) × 6
Sr—O^{ii}	2.622 (4) × 2	Cd—Pt	2.89837 (18) × 2
Sr—O^{iii}	2.635 (4) × 2	Pt—O	2.039 (4) × 6
Sr—O^{iv}	2.739 (4) × 2		

Symmetry codes: (i) $-x+y, -x, z$; (ii) $\frac{2}{3}+x-y, \frac{1}{3}+x, \frac{1}{3}-z$; (iii) $\frac{2}{3}-y, \frac{1}{3}+x-y, \frac{1}{3}+z$; (iv) $\frac{2}{3}-x, \frac{1}{3}-y, \frac{1}{3}-z$.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.072
S = 1.086
505 reflections
19 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2 + 3.1434P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 5.05 e Å^{-3}
$\Delta\rho_{min}$ = −3.56 e Å^{-3}

Systematic absences in the data sets for both compounds confirmed a c glide operation, indicating the space groups $R3c$ and $R\bar{3}c$. Preliminary powder X-ray diffraction showed the compounds to be isostructural with K_4CdCl_6 (space group $R\bar{3}c$); therefore, the expected centrosymmetric space group was chosen and confirmed by the solution. The largest difference peaks were both located less than 0.8 Å from the Zn or Cd atoms. The relatively large values of $\Delta\rho_{max}$ in the vicinity of Zn^{I} and Cd^{II} suggest a small fraction of these atoms may be located off the threefold axis. However, refinement of the Zn or Cd site-occupancy factors for each structure did not lead to a significant deviation from unity and refinements including off-axis contributions were unstable.

For both compounds, data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: BR1306). Services for accessing these data are described at the back of the journal.

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